2P073 MuSTAR MD : Multi-Scale Temperature Accelerated Replica exchange Molecular Dynamics

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We developed a new sampling method, MuSTAR MD which is an extension of temperature accelerated MD and can also be considered as a variation of replica-exchange MD. In the MuSTAR MD, each replica contains an all-atom model, at least one coarse-grained model, and a collective variable model that interacts with the other models through coupling terms. The coarse-grained model is introduced to drive efficient sampling of large conformational space and the all-atom model can serve to conduct accurate conformational sampling. The coupling strengths are exchanged between neighboring replicas in some interval obeying the Metropolis method. MuSTAR MD was applied to Ala-dipeptide and met-enkephalin. Comparison with existing methods shows the efficiency and accuracy of MuSTAR MD.

**2P074 α -シヌクレイン繊維形成に対する分子混雑の影響
Macromolecular crowding effect on fibril formation of α -synuclein**

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An aggregated form of α -synucleins are found in the Lewy body, which is the pathological hallmark of Parkinson's disease. The native state of α -synucleins are in a stable α -helical tetrameric state, while their monomeric state is disordered state. An *in vitro* experiment showed that fibril formation of α -synucleins occurs in their disordered state. These fibrils are considered as seeds for the aggregated form. In order to investigate the mechanism of transition from stable tetrameric state to monomeric disordered state, we constructed a simple lattice gas model considering the effects of macromolecular crowding. We found that decrease of macromolecular density causes tetramer-monomer transition and leads to subsequent fibril formation.

**2P075 サルモネラべん毛繊維の多型変換におけるフラジェリン Arg 431 の役割
The role of Arg431 of flagellin in the polymorphic transformation of Salmonella flagellar filament**

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Salmonella flagellar filament is a μm -length scale and helical structure composed of $\sim 30,000$ molecules of a single protein flagellin. The filament transforms among several helical structures, which are different in curvature and twist, and the morphological transformation is called polymorphic transformation. Elucidating the atomic mechanism of the transformation observed at μm scale provides a new insight into the actuating mechanism of large protein machines. Previously, we proposed that Arg431 of flagellin is one of the key residues for the polymorphic transformation by *fliC*-intragenic suppressor analysis. In the present study, we created mutants carrying mutations at Arg431 and investigated their filament shape and polymorphic transformation activity.

**2P076 表面力測定によるシグナル伝達タンパク質間相互作用の研究
Interactions between signal transduction proteins studied by surface forces measurement**

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Spoluation in *Bacillus subtilis* is controlled by phosphorelay signal transduction. In this series of phosphorylation reactions, KinA binds ATP and autophosphorylates at a histidine residue (KinA-P). The phosphoryl moiety on KinA is transferred to Spo0F and then to Spo0B. We have succeeded in measuring the specific interactions between KinA and Spo0F only in the presence of ATP by using colloid probe AFM. In this study, we focused on the second step of the series of phosphorylation reactions. Proteins were immobilized on a glass substrate using Langmuir Blodgett films of a chelate amphiphile. The conditions of absorbing proteins were determined using quartz crystal microbalance. We measured the interactions between Spo0F and Spo0B in buffer solution with/without KinA-P.

**2P077 X線自由電子レーザーにより得られる低分解能データセット
に対する単粒子構造解析法
Methodology of a single biomolecular structure determination
for low-resolution data set obtained by X-ray Free Electron
Laser**

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X-ray Free Electron Laser offer new possibility of the single biomolecular structure determination. In experiment, bright coherent X-ray pulse is irradiated onto a single biomolecule with unknown orientation, and diffraction patterns are recorded repeatedly for 3D structure. However, in the current status, we can obtain only low resolution data set because of the absence of efficient sample delivery system. Therefore, we are developing a methodology for structure determination using currently attainable data set. To compensate low resolution data set, we assume structure models from simulation and perform diffraction pattern matting by using a similarity detection algorithm (Tokuhisa et al., 2012, Acta Cryst A. 68. 336-381). We report current status of our effort.

**2P078 圧縮センシングを用いた NMR スペクトルの復元法
Reconstruction of NMR spectra using compressed sensing**

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NMR spectroscopy is a non-destructive technique used to reveal structural information of molecules, including biomolecules in solution. Since the invention of multidimensional NMR spectroscopy, the area of its application in structural biology has been growing, and the current interest reached as far as using it to inspect proteins in a living cell. But the largest obstacle for its realization is the severe requirement for measurement time; it has to be much shorter than those of usual cases due to the deterioration of a cell.

To solve the problem, we attempted using compressed sensing theory, a cutting-edge theory for reconstructing data from thinned-out sampling points, to achieve shorter measurement time by measuring with much less sampling points.